MM 25: Interface Controlled Properties, Nanomaterials, and Microstructure Design I

Time: Wednesday 15:45–17:00 Location: SCH/A215

MM 25.1 Wed 15:45 SCH/A215

Confined but Active: Atomic-Scale Dynamics of Gallium and Silver Intercalation in Graphene/SiC — •Nadire Nayir[1], Qian Mao[2], Malgorzota Kowalik[2], and Adri van Duin[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]The Department of Mechanical Engineering, The Pennsylvania State University, PA, US

Metal intercalation at the interface of epitaxial graphene and SiC offers a powerful approach for stabilizing covalently bonded materials in two dimensional form [1-2]. This talk focuses on the atomic-level modeling of 2D metals (i.e. Ga and Ag) grown via confinement heteroepitaxy [2]. The intercalation mechanisms differ notably between metals. Combined photoemission electron microscopy and multiphysics simulatiosn reveal that while metal de-intercalation emerge in all cases, their re-intercalation dynamics vary markedly. For Ag, reversible de- and re-intercalation occurs through defects. In contrast, Ga exhibits irreversible de-intercalation characterized by faster kinetics. Multiphysics simulations integrating ReaxFF and Density functional theory simulations uncover the origin of these distinct behaviors, showing that Ga atoms bind more strongly to graphene than Ag atoms consistent with the faster, irreversible diffusion kinetics observed experimentally. Overall, the findings highlight that both the thermophysical properties of the intercalated metal and its interactions with defective graphene critically determine the intercalation behavior. [1] Nature materials 19 (6), 637-643(2020) [2] Small 20 (11), 2306554(2024)

MM 25.2 Wed 16:00 SCH/A215

Accelerating grain boundary segregation studies in ferritic steels with machine learned interatomic potentials — •Han Lin Mai[1], Tilmann Hickel[2], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials GmbH, Dusseldorf, Germany — [2]BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The segregation of solute and impurities to grain boundaries (GBs) can critically alter the mechanical properties of steels. To predict segregation phenomena, ab-initio methods such as density functional theory (DFT) are frequently used, but their computational expense limits the size of the model GBs viable for computation. This limitation has rendered access to segregation statistics out of reach and therefore has hindered our understanding of segregation phenomena. Here, we present a machine learned interatomic potential (MLIP) for multiple Fe-X binary alloys that predict segregation energies approaching ab-initio accuracy with automated dataset generation techniques. We use these potentials to conduct high-throughput segregation studies to generate segregation energy spectra and compare these to those commonly found in GBs accessible to DFT studies. Commonly purported relationships between GB quantities such as excess volume, site volume and GB energies and the strength of segregation binding of solutes and impurities are re-examined and revised.

MM 25.3 Wed 16:15 SCH/A215

Defect Phase Diagrams for Exploring Chemo-Structural Coupling in Ni Grain Boundaries — •Prince Mathews[1], Ali Tehranchi[1], Jörg Neugebauer[2], and Tilmann Hickel[1,2] — [1]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany — [2]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The knowledge-driven framework of defect phase diagrams (DPDs) offers an effective and systematic approach to design materials with tailored properties. Unifying bulk and defect thermodynamics along with the consideration of structural and chemical complexities around defects, DPDs advance the fundamental understanding of defects and can also provide a pathway for guided microstructure design. In this work, we apply the framework of DPDs using ab-initio calculations to evaluate the stability of defect phases and investigate defect phase transformations in Ni grain boundaries. In competition with the nearest intermetallic phase, Nb containing defect phases are stable in $\Sigma5$ [001]/(310) whereas Nb containing defect phases are not stable in $\Sigma3$ [110]/(111) grain boundaries. Moreover, our findings indicate the preference of solutes to segregate at sites around defects with partial column occupations. Furthermore, with the application of a sub-lattice based model, we present the insights on grain boundary site column coverages as a function of temperature. In addition, we discuss a new approach for determining a characteristic defect width using the solute distribution probability across the defect which facilitates the integration of defects into the CALPHAD methodology.

MM 25.4 Wed 16:30 SCH/A215

Non-Hermitian physics and exceptional points at Z2 Weyl semimetal*ferromagnet junctions — •Tong Wang[1], Robert Amelung[2], and Flore Kunst[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Non-Hermitian systems extend beyond the framework of Hermitian quantum mechanics and allow for the description of open systems with loss and gain. The study of non-Hermitian physics leads to an enrichment of topological phases of matter and practical applications in photonics and sensing. Here we study the junction between a metallic ferromagnet and a Z2 Weyl semimetal [1], where a combined time-reversal symmetry and reflection symmetry leads to degenerate helical Fermi arcs on certain surfaces. The couplings at the material interface give arise to a complex self-energy in the Green's function [2], rendering the effective Hamiltonian of the Fermi arc surface states non-Hermitian. We show that non-Hermiticity can break a degenerate Fermi arc into pairs of exceptional point, and the resulting exceptional phase persists for a wide parameter range regarding the magnetization of the ferromagnet and topological mass term of the semimetal. We also discuss the how the exceptional points may influence physical properties of the Z2 Weyl semimetal. [1] T. Morimoto and A. Furusaki, Phys. Rev. B 89 235127 (2014). [2] E. J. Bergholtz and J. C. Budich, Phys. Rev. Res 1 012003(R) (2019).

MM 25.5 Wed 16:45 SCH/A215

Theory Unravels Electro-Ionic Metal-Support Interactions at Supported Electrocatalyst Nanoparticles — •Yufan Zhang, Tobias Binninger, Jun Huang, and Michael Eikerling — Theory and Computation of Energy Materials, Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Electrochemical energy conversion requires electrocatalysts to accelerate reactions. Most theoretical studies used idealized planar electrodes, whereas real catalysts typically consist of supported nanoparticles (NPs) with heterogeneous compositions and structures that lead to unique electronic and ionic properties.

In this talk, I will present results from our recently published paper [1]. Using density-potential functional theory, we calculate the contact electrification of a Ag NP and a Au support. While traditional view believes that electron redistribution is confined to the NP-support contact interface, we reveal that it also occurs at the NP's external surface, directly influencing the catalytically active sites. The electron redistribution generates an electric field in electrolyte surrounding the supported NP, which further leads to ion separation. The support-induced charge perturbations at the NP's external surface can be no longer described by the classical concept of the potential of zero charge for planar electrode. To address this, we define a global and two local characteristic potentials. It is demonstrated that the electronic and ionic effects are strongly coupled at supported NPs, and are therefore best described as electro-ionic metal-support interactions (EIMSI).

[1] Y. Zhang, et al., Phys. Rev. Lett. 134, 066201 (2025).